1. State the two Schrödinger equations for electrons in a periodic potential field (Kronig-Penny model). Use for their solutions, instead of the Bloch function, the trial solution $\Psi(x) = A e^{ikx}$

Discuss the result. (*Hint*: For free electrons $V_o = 0$)

S.E. I (no potential) : $\frac{d^2\Psi}{dx^2} + \frac{2mE}{\hbar^2}\Psi = 0$

S.E. II
$$(v=v_0)$$
: $\frac{d^2\Psi}{dx^2} + \frac{2m(E-v_0)}{\hbar^2}\Psi = 0$

The trial solution $\Psi(x) = Ae^{ikx}$ $\Pi \stackrel{\circ}{\exists}$. $(\frac{d\Psi}{dx} = A_i e^{ikx}, \frac{d^2\Psi}{dx^2} = -Ak^2 e^{ikx})$

I:
$$-Ak^2e^{ikx} + \frac{2mE}{\hbar^2}Ae^{ikx} = 0$$
 $\therefore k^2 = \frac{2mE}{\hbar^2}$

II:
$$-Ak^{2}e^{ikx} + \frac{2m(E-v_{0})}{\hbar^{2}}Ae^{ikx} = 0$$
 $\therefore k^{2} = \frac{2m(E-v_{0})}{\hbar^{2}}$ $v_{0} = 0$

Bloch function $\Psi(x) = u(x) \cdot e^{ikx}$ 에서 u(x)는 lattice의 peridicity를 알려주는 주기함수이다. u(x)가 constant A일 경우 periodic potential이 없는 $(v_0 = 0)$ 상황이 되어 free electron과 같은 경우가 된다.

2. The differential equation for an undamped vibration is $a\frac{d^2u}{dx^2} + bu = 0$ (1) whose solution is $u = Ae^{ikx} + Be^{-ikx}$ (2) Where $k = \sqrt{b/a}$ Prove that (2) is indeed a solution of (1) $u = Ae^{ikx} + Be^{-ikx}$ (2) $a\frac{d^2u}{dx^2} + bu = 0$ (1) $k = \sqrt{b/a}$

$$\begin{split} &(2) \stackrel{i}{\ominus} \stackrel{i}{\ominus} (1) \stackrel{i}{\ominus} \stackrel{i}{\Box} \\ &\frac{du}{dx} = A_i k e^{ikx} - B_i k e^{-ikx}, \qquad \frac{d^2 u}{dx^2} = -A_i k^2 e^{ikx} - B_i k^2 e^{-ikx} \\ &\therefore a \cdot \left(-A_i k^2 e^{ikx} - B_i k^2 e^{-ikx} \right) + b \left(A e^{ikx} + B e^{-ikx} \right) \\ &= \left(-aA \cdot \frac{b}{a} + bA \right) e^{ikx} + \left(-aB \cdot \frac{b}{a} + bB \right) e^{-ikx} = 0 \end{split}$$

3. The total electron energy of a hydrogen atom is given by

$$E = \frac{me^4}{2(4\pi\varepsilon_0\hbar)^2} \frac{1}{n^2} = -13.6 \cdot \frac{1}{n^2} (eV)$$

where n = 1, 2, 3, ...

(a) Derive the above relation in a semiclassical way by assuming that the centripetal force of an electron, mv^2/r , is counterbalanced by the Coulombic attraction force,

 $-e^2/4\pi\varepsilon_0 r^2$, between the nucleus and the orbiting electron. Use Bohr's postulate which states that the angular momentum L = mvr (v = linear electron velocity and r = radius of the orbiting electron) is a multiple integer of Planck's constant (i.e., $n\hbar$). (*Hint*: The kinetic energy of the electron is $E = mv^2/2$)

$$\begin{split} F &= \frac{mv^2}{r} = \frac{e^2}{4\pi\epsilon_0 r^2} \qquad (\forall \vec{v} \ \vec{v} \ \vec{z} \ \vec{d} \ \vec{+} \ \vec{z} \ \vec{d} \ \vec{v}, \qquad v^2 = \frac{e^2}{4\pi\epsilon_0 mr} \\ Bohr's postulate \qquad L &= mvr = n\hbar, \quad r = n\hbar/mv \qquad v^2 = \\ \frac{e^2 mv}{4\pi\epsilon_0 mn\hbar} \\ E &= KE + PE \ (PE = -\int F(r)dr = -e^2/4\pi\epsilon_0 r) \\ &= \frac{1}{2}mv^2 - \frac{e^2}{4\pi\epsilon_0 r} = \frac{1}{2}mv^2 - mv^2 = -\frac{1}{2}mv^2 = -\frac{m}{2} \cdot \frac{e^4}{(4\pi\epsilon_0 r)^2} \cdot \frac{1}{n^2} \\ &= \frac{-9.11 \times 10^{-31} \times (1.6 \times 10^{-19})^4}{2 \times (4\pi \times 8.85 \times 10^{-12} \times 6.626 \times 10^{-34}/2\pi)^2} \cdot \frac{1}{n^2} = -2.17 \times 10^{-18} \cdot \frac{1}{n^2} (J) \\ &= -13.6 \cdot \frac{1}{n^2} (eV) \end{split}$$

(b) Derive the above relation by solving the Schrodinger equation for the electron wave of the hydrogen atom.

(Hint, refer to Concepts of Modern Physics, Ed. Arthur Beiser or other books) (hydrogen atom.pdf 파일 첨부)

- 4. Consider an electron trapped in a one-dimensional box with infinitely high potential. The box extends from x = 0 to x = a. The electron has the mass *m* and the total energy *E*.
- (a) Find the energy eigenvalue of the electron by solving Schrödinger equation,

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}E\psi = 0$$

 $\frac{d^2\Psi}{dx^2} + \frac{2mE}{\hbar^2} E\Psi = 0 \quad k = \frac{\sqrt{2mE}}{\hbar}, \ \frac{d^2\Psi}{dx^2} = -k^2 \Psi$

Ψ = Asinkx + Bcoskx (Ae^{ikx} + Be^{-ikx}와 같은 형태) x=0 에서 Ψ = 0, ∴Ψ(0) = B = 0 x=a 에서 Ψ = 0, ∴Ψ(a) = Asinka = 0, A≠0이어야 물리적 의미를 가지므로 ka=nπ (n=1, 2, 3...)

$$\therefore k = \frac{n\pi}{a}, \quad E_n = \frac{\hbar^2 k^2}{2m} = \frac{n^2 \pi^2 \hbar^2}{2ma^2} \quad (n = 1, 2, 3 ...)$$

(b) If the lowest energy possible for the electron is 10.00 eV, what are the two higher energies the particle can have?

The lowest energy: 10.00eV (n=1)

The two higher energies: $E_n \propto n^2$ 이므로 $E_2 = 40.00 \text{eV}, E_3 = 90.00 \text{eV}$

(c) Find the eigenfunction ψ_n corresponding to E_n .

(c)
$$f_{\mu} = A \sin \frac{1}{2} = A \sin \frac{n\pi x}{a}$$
, normalization : $\int_{-\infty}^{\infty} |\psi_{\mu}|^{2} dx = 1$
 $\int_{-\infty}^{a} A^{2} \sin^{2} \frac{n\pi x}{a} dx = A^{2} \int_{0}^{a} \left(\frac{1}{2} - \frac{1}{2}\cos\frac{2n\pi x}{a}\right) dx$
 $= A^{2} \left|\frac{1}{2}x - \frac{1}{2}\frac{a}{2n\pi c}\sin\frac{2n\pi x}{a}\right|_{0}^{a} = A^{2} \cdot \frac{a}{2} = \frac{1}{2}$, $A = \int_{a}^{2} \frac{1}{a}$
 $\therefore f_{\mu} = \int_{a}^{2} \sin \frac{n\pi x}{a}$

(d) Find the probability density that the electron can be found between x = 0 and a/3 for the second excited sate (n = 3).

(d) the probability density
$$(0 \langle \chi \leq \frac{\alpha}{3} \rangle \Rightarrow \int_{0}^{\frac{\alpha}{3}} |\frac{1}{3}|^{\frac{\alpha}{2}} dx \quad (n=3)$$

$$\int_{0}^{\frac{\alpha}{3}} \frac{2}{\alpha} \sin^{2} \frac{3\pi \chi}{\alpha} dx = \frac{2}{\alpha} \int_{0}^{\frac{3}{3}} \left(\frac{1}{2} - \frac{1}{2}\cos\frac{6\pi \chi}{\alpha}\right) dx$$

$$= \frac{2}{\alpha} \cdot \left|\frac{1}{2}\chi - \frac{\alpha}{12\pi}\sin\frac{6\pi \chi}{\alpha}\right|_{0}^{\frac{\alpha}{3}} = \frac{\beta}{\kappa} \cdot \frac{1}{\gamma} \frac{\alpha}{3} = \frac{1}{3}$$

5. An electron of mass m and kinetic energy E > 0 approaches a potential drop V_0

(a) Write down the equations of two regions (x≥0, x≤0) from time-independent Schrödinger equation.

(b) Assume there is no incoming wave to the right, so you can get three amplitude constants. Let A : incident amplitude, B : reflected amplitude, C : transmitted amplitude.

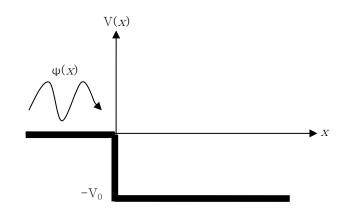
Determine the reflection coefficient *R*. $(R = \frac{|B|^2}{|A|^2})$

$$(b) \ x \leq 0$$

$$k_{1} = \frac{\int \lambda_{m}E}{k}, \ f_{1}(x) = A e^{\lambda kx} + B e^{\lambda kx}$$

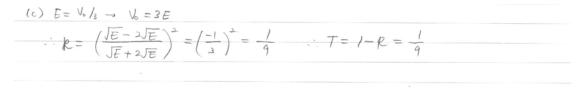
$$T_{-}, \text{ reflected amplitude}$$

$$T_{-}, \text{ reflected$$



(c) What is R if $E = V_0 / 3$?

Calculate the transmission coefficient *T* in this case from R + T = 1.



6. For an electron in a one dimensional crystal, assuming it experiences one dimensional periodic potential (Kronig-Penny model) shown below, $(E < V_0)$

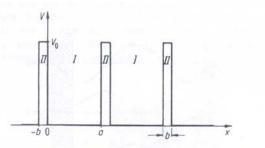


Figure 4.9. One-dimensional periodic potential distribution (simplified) (Kronig-Penney model).

(a) Using the Bloch function $\psi(x) = u(x) \cdot e^{ikx}$ as the wave function of the electron, show that solution of the Schrodinger equations in regions I and II leads to

$$\frac{\gamma^2 - \alpha^2}{2\alpha\gamma} \sinh(\gamma b) \cdot \sin(\alpha a) + \cosh(\gamma b) \cdot \cos(\alpha a) = \cos k(a+b)$$

Where, $\alpha^2 = \frac{2m}{\hbar^2} E$ $\gamma^2 = \frac{2m}{\hbar^2} (V_0 - E)$

9 (o) Kronig-Penny model (E
(1)
$$\frac{d^{2}u}{dx^{2}} + \frac{2m}{t^{2}}E^{4} = 0$$

(2) $\frac{d^{2}u}{dx^{2}} + \frac{2m}{t^{2}}E^{4} = 0$
(3) $\frac{d^{2}u}{dx^{2}} + \frac{2m}{t^{2}}E^{4} = 0$
(4) $\frac{d^{2}u}{dx^{2}} + \frac{2m}{t^{2}}(E-V)^{\frac{1}{2}}=0$
 $\alpha^{2} = \frac{2mE}{t^{2}}, \ \delta^{*} = \frac{2m}{t^{2}}(U-E)^{-\frac{1}{2}}+\frac{\pi}{t^{2}}+\frac{\pi}{t^{2}}$
(1) $\frac{d^{2}u}{dx^{2}} + 2a_{k}\frac{du}{dx} - (k^{2}-a^{2})u = 0, \ (2)\frac{d^{2}u}{dx^{2}} + 2a_{k}\frac{du}{dx} - (k^{2}+b^{2})u = 0$
 $2^{\frac{1}{2}t^{2}} \frac{2^{\frac{1}{2}t}}{dx^{2}} + 2a_{k}\frac{du}{dx} - (k^{2}-a^{2})u = 0, \ (2)\frac{d^{2}u}{dx^{2}} + 2a_{k}\frac{du}{dx} - (k^{2}+b^{2})u = 0$
 $2^{\frac{1}{2}t^{2}} \frac{2^{\frac{1}{2}t}}{dx^{2}} \frac{\pi}{t^{2}}+\frac{\pi}{t^{2}}$
(1) $u = e^{-\frac{1}{2}kx}\left(Ae^{\frac{1}{2}tx} + 8e^{-\frac{1}{2}tx}\right), \ (2) u = e^{-\frac{1}{2}kx}\left(Ce^{-\frac{1}{2}tx} + 2e^{\frac{1}{2}k}\right)$
Boundary condition $\frac{\pi}{t^{2}} - \frac{2^{\frac{1}{2}t}}{t^{2}}+\frac{\pi}{t$

n.(a) Kronig - Penney mod	$el \rightarrow four eq$	wations		
\bigcirc A+B = C+D				
@ A (id-ik) +B fid-	r(k) = C(-r - r)	$ik) + D(\sigma - ik)$		
3 Ae(1 d- = k) a + Be (-= a				
			(ik+o)b	(ik-+)b
$(a \land (a - k) e^{ia(a - k)} - $	Bridtk)C	$= -C(\delta + ik)$	$e^{-1} + D(\delta - \delta)$	-ik)e
-> 4740/ yer A.B.	C. D 24 → A	.B.C.D =1 alit 4×4	+ matrix = 743	for det=0 ==
반록지키는 관계 성을 3	रिल्ल खुल			
비사은 행전도 포현	1 /	1	-1	1
det	id-ik	-id -ik $e^{(-iu-ik)a}$ e^{i} $-i(dtk)e^{-ia(uti)}$	d+zk -e(ik+o)b	-d+:k
1対:①	e con appa	erration	-e	- e"+ "
ンゴリ: ② 3799: ③	= (d-)e e ala-	- = (dtk) e = = = = = = = = = = = = = = = = = =	+(d+ik)C	$\frac{16}{-(\delta-ik)e^{(ik-\delta)b}}$
4號 @	= 0			
가 했이 상수는 문화에 구	기도 곳은 한 것	는 상수에 하여 다는 해	lon tished 5 det ()=0 the stal of
(행관 순서는 바구에도				
Dx b + D	· · · · · · · · · · · · · · · · · · ·	-> M3-3 2= (Q')		
Oxik+B ide"	(x-k) -ide -ia	lotth) J-C(sk+d)b	-re(ik-+)b ->	@'
		- e = (0+6) & + + + b		
@'x eiba id e ind				
· · · · · · · · · · · · · · · · · · ·	3 2 2 2 2	ide ina -ide in	a de slotbiktob	-de = (orb)k-ob
0	,) ⇒ (ide ^{ida} -ide ^{ida} e ^{ida} e ^{-ida} id -id	- C = (otb)k++b	-e = (++)k-ob
0	/	id -id	8	-8
		1 1	-1	-1 /_
; (otb) k = t 3 刘柱	/ ide ida	$-ide^{-ida}$ de^{t+} e^{-ida} $-e^{t+ab}$ -id d	+b -det-bb	
de	t enda	e-ina -et++b	-et-rb	
	id	rid d	- 2 /	
	1 /	/ _	-1 /	

1)
$$\lambda \alpha \in i^{d\alpha} \times det \begin{vmatrix} e^{-id\alpha} & -e^{itdb} & -e^{itdb} \\ -id & \alpha & -d \\ i & -1 & -1 \end{vmatrix} \qquad \left(\begin{pmatrix} e^{id} + e^{id} + ide - ide + ide +$$

(b) Describe in what condition, the above relation becomes

$$P\frac{\sin\alpha a}{\alpha a} + \cos\alpha a = \cos ka \quad \text{where} \quad P = \frac{maV_0b}{\hbar^2}$$

$$P\frac{\sin\alpha a}{\alpha a} + \cos\alpha a = \cos ka \quad \text{where} \quad P = \frac{maV_0b}{\hbar^2}$$

$$P\frac{\sin\alpha a}{\hbar^2} \sin h(\delta b) \cdot \sin(\delta a) + \cosh(\delta b) \cdot \cos(\delta a) = \cosh(\delta b)$$

$$\frac{\partial^2 - \alpha^2}{\partial \alpha^2} \sin h(\delta b) \cdot \sin(\delta a) + \cosh(\delta b) \cdot \cos(\delta a) = \cosh(\delta b)$$

$$\frac{\partial^2 - \alpha^2}{\partial \alpha^2} \sin b \cdot \sin(\delta a) + \cos(\delta a) = \cosh(\delta b) \sin(\delta b) \sin(\delta b) = \frac{\partial^2 - \alpha^2}{\partial \alpha^2} \sin b \sin(\delta b) = \frac{\partial^2 - \alpha^2}{\partial \alpha^2} \sin b \sin(\delta b) = \frac{\partial^2 - \alpha^2}{\partial \alpha^2} \sin b \sin(\delta b) = \frac{\partial^2 - \alpha^2}{\partial \alpha^2} \sin b \sin(\delta b) = \cos(\delta a)$$

$$P = \frac{maV_0b}{\hbar^2} \sin(\delta a) + \cos(\delta a) = \cosh(\delta b) = \cos(\delta a)$$

$$P = \frac{maV_0b}{\hbar^2} \sin(\delta a) + \cos(\delta a) = \cosh(\delta a) = \cos(\delta a)$$